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# Remarks on causality, localization, and spreading of wave packets

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Localization properties of general quantum systems and their connection with causality are studied, extending previous results by the first-named author.

## I. INTRODUCTION

For a free nonrelativistic wave packet it is well known that it spreads instantaneously over all of space if it is localized in a bounded region at time $t=0$. For a free relativistic particle the meaning of localization is not quite clear *a priori*, but, for example, for the Newton-Wigner position operator a similar phenomenon occurs[1] and it also occurs in some models in which localization is expressed by means of a current density four-vector.[2] For relativistic particles there is a host of other position operators that have been proposed.[3] However, if one only assumes that one-particle states localized in disjoint regions are orthogonal to each other, then, as was shown by one of us,[4] a particle will spread infinitely fast if initially confined in a bounded region of space; this result was later generalized to relativistic many-particle systems by means of the edge-of-the-wedge theorem.[5] It was not shown in Refs. 4 and 5, however, that the spreading was over *all* of space. These results imply, of course, that one runs into conflict with (Einstein) causality—no propagation faster than the speed of light—as soon as one *can* localize particles in a bounded region.

In Secs. II A and II B of this paper we use very simple analyticity arguments to first extend the results of Refs. 4 and 5 to a quite general class of time evolutions, not just relativistic ones. One only needs a very weak condition on the energy-momentum spectrum; for instance, if the energy is a function $\omega(\underline{P})$ of momentum, as for a single particle, then it suffices that $\omega \geq -c$ and that $\omega$ is not identically constant. Under slightly stronger assumptions it is then shown in Sec. II C that, if $V$ is any (bounded or unbounded) open region of space and if the system is initially outside $V$, it will be immediately afterwards everywhere in $V$. Pictorially this means that a wave function cannot exhibit "holes" for finite-time intervals.

In Sec. II we make essential use of the assumption that space and time translations commute. Thus, we have restricted ourselves to translation-invariant systems in this section. In the case of many-particle systems one may also ask whether results of this nature hold for translations of the relative coordinates. Similar questions arise for particles in external potentials. Such systems are discussed in Sec. III.

The proofs of Theorems 2.1 and 2.2 below use the physicist's language of non-normalizable eigenvectors and are basically quite simple. For the more mathematically inclined reader we have added an appendix where these results are slightly extended and proved by using the spectral theorem. In this appendix we have also included another result requiring more mathematical background than the main text. This result concerns the absence of compact localization of states in the continuous spectrum of the Hamiltonian for a particle in an external potential.

## II. TRANSLATION-INVARIANT SYSTEMS

In this section we consider a physical system described by a Hilbert space $\mathcal{H}$ and a time development operator $U_t = \exp(-iHt)$ with self-adjoint Hamiltonian $H$. One may think of $N$ interacting or noninteracting particles, $N \geq 1$. It is assumed that there are unitary operators $U(\underline{a})$, $\underline{a} \in R^3$, corresponding to space translations, i.e., if some state of the system is described by some $\phi \in \mathcal{H}$ then the translated state is described by $U(\underline{a})\phi$. One can write $U(\underline{a}) = \exp(-i\underline{P}\cdot\underline{a})$. $H$ and $\underline{P}$ are conventionally identified with the energy and momentum operators of the system. We assume that the Hamiltonian is translation invariant, i.e.,

$$[H, \underline{P}] = 0, \quad [U_t, U(\underline{a})] = 0 \quad \text{for all } t, \underline{a}. \tag{2.1}$$

This means that $H$ and $\underline{P}$ can be diagonalized simultaneously with in general non-normalizable eigenvectors.[6] The set $(p^0, \underline{p})$ of all (generalized) eigenvalues of $(H, \underline{P})$ is the energy-momentum spectrum or joint spectrum. For a one-particle system $H$ will be a function of $\underline{P}$, $H = \omega(\underline{P})$, so that $p^0 = \omega(\underline{p})$, and hence the energy-momentum spectrum will be a surface in $R^4$. If $H$ is not a function of $\underline{P}$, as for interacting many-particle systems, the spectrum is more general. For instance, for a system of particles with masses $m_1, \ldots, m_N$ that interact through positive pair potentials the spectrum is the set of $(p^0, \underline{p}) \in R^4$ satisfying $p^0 \geq \underline{p}^2/2M$ or $p^0 \geq (\underline{p}^2+M^2)^{1/2}$ (where $M \equiv \sum_{i=1}^N m_i$), if the system is described in a nonrelativistic or relativistic framework, respectively (cf. also remarks 4 and 5 in Sec. II C). For a general relativistic system, as in quantum field theory, one has $p^0 \geq |\underline{p}|$.

The Hamiltonian is bounded from below, $H \geq -c > -\infty$, if all $p^0$ values satisfy $p^0 \geq -c$. This is equivalent to $\langle \phi, H\phi\rangle \geq -c$ for all $\phi$ in the domain of $H$. If $H \geq -c$ one can assume $c=0$ by adding a constant to $H$.

### A. A consequence of positive energy

Positivity of the energy has a simple but important consequence whose proof is based on an elementary analyticity argument.

*Lemma.* Let $H \geq -c$. Let $\mathcal{H}'$ be a closed subspace of $\mathcal{H}$ and assume that for some $\psi \in \mathcal{H}$ and some open time interval $I$, $U_t\psi \in \mathcal{H}'$ for any $t \in I$. Then $U_t \psi \in \mathcal{H}'$ for any $t \in R$. More generally, if $A$ is a bounded operator and $AU_t\psi=0$ for any $t \in I$, then $AU_t\psi = 0$ for any $t \in R$.

*Proof.* Let $\phi$ be an arbitrary vector orthogonal to $\mathcal{H}'$. Let $z=t+iy$ with $y \leq 0$. Then

$$g(z) \equiv \langle \phi, \exp(-iHz)\psi\rangle \tag{2.2}$$

is analytic for $y<0$ since $H \geq -c$. Moreover, $g(z)$ is continuous for $y \leq 0$ and vanishes for $z=t\in I$. But then $g(z)$ vanishes for all $z$ by the Schwarz reflection principle.[7] This implies that $\phi$ is orthogonal to $U_t\psi$ for all $t \in R$, i.e., the first part of the lemma. The second part follows in the same way by taking $\phi = A^*\chi$ with an arbitrary $\chi \in \mathcal{H}$. Q.E.D.

Another way of stating the first part of the lemma is that the subspace spanned by $\{U_t\psi; t\in[a,b]\}$ for given $\psi$ and $a<b$ is invariant under all $U_t$ (it may coincide with $\mathcal{H}$).

### B. Instantaneous spreading from bounded regions

Using the lemma just proved we shall now discuss the spreading of wave packets. Assume that for a system in a state $\psi$ a notion of localization is given. As in Refs. 4 and 5 we assume at this point only that, if $\psi$ and $\phi$ are localized in regions far apart, $\psi$ is orthogonal to $\phi$. This will be further motivated in Sec. II C. Now let $U_t\psi$ be localized in a bounded region $V$ for $0 \leq t \leq \epsilon$. Then $U(\underline{a})\psi$, the translate of $\psi$, should be localized outside $V$ for $|\underline{a}|$ sufficiently large, and hence for some $r>0$

$$\langle U(\underline{a})\psi, U_t\psi\rangle = 0 \quad \text{for any } 0 \leq t \leq \epsilon, \quad |\underline{a}| \geq r. \tag{2.3}$$

The following theorem shows that this assumption implies that $\psi = 0$, provided some spectral conditions are met.

*Theorem 2.1* ("no bounded localization"). Let $U(\underline{a})$ and $U_t$ commute and let $H \geq -c$. Assume there exists a sequence of finite disjoint intervals $I_k \subset R$ $(k=1,2,\ldots)$ such that

(i) the union $\cup_{k=1}^{\infty} I_k$ contains the energy spectrum;

(ii) for each $k$ there is an open set $O_k \subset R^3$ such that $I_k \times O_k$ is not contained in the energy-momentum spectrum.

Finally, assume that $\psi \in \mathcal{H}$ satisfies the condition (2.3). Then $\psi = 0$.

*Proof.* Since $H$ is bounded from below the lemma implies that Eq. (2.3) holds for all $t \in R$ if $|\underline{a}| \geq r$. For any of the above $I_k$, let $\chi_{I_k}(p^0)$ be 1 on $I_k$ and zero outside. Then one also has[8]

$$\langle U(\underline{a})\psi, \chi_{I_k}(H)\psi\rangle = 0 \quad \text{for } |\underline{a}| \geq r. \tag{2.4}$$

Now $\psi_k \equiv \chi_{I_k}(H)\psi$ contains only energy values in $I_k$ and, by condition (ii), only momentum values outside the set $O_k$. In the momentum representation $\psi_k \sim \psi_k(\underline{p})$,[9] one then has $\psi_k(\underline{p}) = 0$ for $\underline{p} \in O_k$. From

$$\begin{aligned} F_k(\underline{a}) &\equiv \langle U(\underline{a})\psi, \chi_{I_k}(H)\psi\rangle \\ &= \int \exp(i\underline{p}\cdot\underline{a})\langle\psi(\underline{p}), \psi_k(\underline{p})\rangle d\mu(\underline{p}), \end{aligned} \tag{2.5}$$

one has

$$\tilde{F}_k(\underline{p})d\underline{p} = \langle \psi(\underline{p}), \psi_k(\underline{p})\rangle d\mu(\underline{p}),$$

where the right-hand side vanishes on $O_k$. But, by Eq. (2.4), $F_k(\underline{p})$ is the Fourier transform of a function of compact support and thus analytic. Hence, if $\tilde{F}_k$ vanishes on $O_k$, $\tilde{F}_k \equiv 0$ and $F_k(\underline{a}) = 0$ for all $\underline{a}$. Since by (i), $\sum_k \chi_{I_k}(H) = 1$, we have

$$0 = \sum_k F_k(\underline{a}) = \langle U(\underline{a})\psi, \sum_k \chi_k(H)\psi\rangle = \langle U(\underline{a})\psi, \psi\rangle$$

for all $\underline{a}$. Putting $\underline{a}=0$ the statement follows. Q.E.D.

*Remarks.*

(1) The theorem implies that a state $\psi_t$ cannot be localized in a finite region $V$ for a finite time interval and that, if initially localized in $V$, it immediately spreads out to infinity under the above spectral assumptions. It need in principle, however, not "cover" all of space. This question will be discussed in Sec. II C.

(2) The spectral assumptions are very weak. If, for example, $H = \omega(\underline{P}) \geq -c$ with $\omega$ continuous, it suffices that $\omega$ is not identically constant on the momentum spectrum.[10] If one only has $H \geq f(\underline{P}) \geq -c$ it suffices that $\sup f(\underline{p}) = \infty$ on the momentum spectrum.

(3) If the energy is not bounded from below one can still obtain information on spreading: Assume that a state $\psi_t$ is localized in $V$ for all $t$ and that (i) and (ii) of Theorem 2.1 hold, but that $H$ is not bounded from below. Then the same argument as before goes through and the analog of Theorem 2.1 would give $\psi_t \equiv 0$ in contradiction to $\|\psi_t\| = 1$.

Hence the state cannot be localized in $V$ for all times. It should be pointed out that in this case instantaneous spreading does not take place in general. For instance, the dynamics given by the free Klein-Gordon and Dirac equations, for which the energy is not bounded from below, give rise to finite propagation speed. An even simpler example is a free particle with "energy" function $\omega(\underline{p})=p_1$. In this case the "time evolution" simply translates the wave packet in the $x_1$ direction.

### C. Absence of holes

In this subsection we assume that some localization operator $N(V)$ for open regions $V\subset R^3$ is given, such that $\langle\phi, N(V)\phi\rangle$ is the probability of detecting the system (or a part thereof, cf. Remark 4 below) in the region $V$, if its state is given by the vector $\phi\in\mathcal{H}$. Since probabilities lie between 0 and 1 we must have

$$0\leqslant\langle\phi, N(V)\phi\rangle\leqslant 1 \quad \text{for } \|\phi\|=1\,. \tag{2.6}$$

This implies that $N(V)$ is self-adjoint. We will say a state $\psi$ is localized in $V$ if the probability of finding it in $V$ is 1, and that it is not in $V$ if the probability is 0. In either case, $\psi$ is an eigenvector of $N(V)$, with eigenvalue 1 and 0, respectively, since

$$1=\langle\psi, N(V)\psi\rangle=\|N(V)^{1/2}\psi\|^2=\|\psi\|^2 \tag{2.7}$$

implies $N(V)^{1/2}\psi=\psi$, and similarly for the second case. Hence, if $\psi$ is localized in $V$, but $U(\underline{a})\psi$ is not in $V$ for some $\underline{a}$, then they are orthogonal. This was used in Sec. II B.

We will make the following two rather weak assumptions, which are physically quite intuitive.

(a) Let $V'\subset V$ be such that the boundaries $\partial V$ and $\partial V'$ have nonzero distance. If $\psi$ is not in $V$ then the translated state $U(\underline{a})\psi$ is not in $V'$ for $|\underline{a}|$ sufficiently small.

(b) For any open region $V$ and state $\psi$ there is a translate $U(\underline{a}_0)\psi$ of $\psi$ that is in $V$ with nonzero probability, i.e.,

$$\langle U(\underline{a}_0)\psi, N(V)U(\underline{a}_0)\psi\rangle\neq 0 \quad \text{for some } \underline{a}_0\,. \tag{2.8}$$

Below we shall give examples of $N(V)$ for which these conditions are satisfied (Remark 4). We are now in a position to state and prove a general result concerning absence of holes.

*Theorem 2.2* ("no holes"). Let $U(\underline{a})=\exp(-i\underline{P}\cdot\underline{a})$ and $U_t=\exp(-iHt)$ commute and let $H\geqslant -c$. Assume there exists a sequence of finite disjoint intervals $I_k\subset R$ $(k=1,2,\ldots)$ and balls $B_k\subset R^3$ such that the union $\cup_k I_k\times B_k$ contains the energy-momentum spectrum.[11]

Now assume there is a state $\psi$ and open region $V_0$ such that $\psi$ is not in $V_0$,

$$\langle\psi, N(V_0)\psi\rangle=0\,. \tag{2.9}$$

Then for any open $V\subset V_0$ and any time interval $(0,\epsilon)$ there is a $t\in(0,\epsilon)$ such that

$$\langle U_t\psi, N(V)U_t\psi\rangle\neq 0\,. \tag{2.10}$$

*Proof.* Assume the statement is incorrect. Then there is some open $V$ and time interval $(0,\epsilon)$ such that

$$\langle\psi_t, N(V)\psi_t\rangle=0 \quad \text{for any } t\in[0,\epsilon]\,. \tag{2.11}$$

Then for any open $V'\subset V$ with $\operatorname{dist}(\partial V,\partial V')>0$ and sufficiently small $|\underline{a}|$, the translated state $U(\underline{a})\psi_t$ is not in $V'$, and thus by the remark following Eq. (2.6),

$$N(V')U(\underline{a})U_t\psi=0 \quad \text{for } t\in[0,\epsilon],\ |\underline{a}|\leqslant\delta\,. \tag{2.12}$$

By the lemma, Eq. (2.11) then holds for all $t$ and also with $U_t\psi$ replaced by $\psi_k\equiv\chi_{I_k}(H)\psi$, as in the proof of Theorem 2.1. The energy values in $\psi_k$ are restricted to $I_k$ and so in the momentum representation, $\psi_k(\underline{p})=0$ for $\underline{p}\notin B_k$. Let $\phi\in\mathcal{H}$ be arbitrary and let $\phi'=N(V')\phi$. Then the function

$$F_k(\underline{a})\equiv\langle N(V')\phi, U(\underline{a})\chi_{I_k}(H)\psi\rangle = \int\exp(-i\underline{p}\cdot\underline{a})\langle\phi'(\underline{p}),\psi_k(\underline{p})\rangle d\mu(\underline{p}) \tag{2.13}$$

is the Fourier transform of a measure of compact support. Hence $F_k(\underline{a})$ is analytic, and since it vanishes for $|\underline{a}|\leqslant\delta$, $F_k(\underline{a})=0$ for all $\underline{a}\in R^3$. Since $\sum_k\chi_{I_k}(H)=1$, we have

$$0=\sum_k F_k(\underline{a})=\langle\phi, N(V')U(\underline{a})\sum\chi_{I_k}(H)\psi\rangle = \langle\phi, N(V')U(\underline{a})\psi\rangle$$

and hence

$$N(V')U(\underline{a})\psi=0 \quad \text{for any } \underline{a}\in R^3\,. \tag{2.14}$$

This contradicts our assumption (b) on $N(V)$, so that the theorem is proved. Q.E.D.

*Remarks.*

(1) The above theorem again implies infinite propagation speed and would thus lead to conflict with causality, unless all physical states were already spread out over all space to start with. This then would rule out that $N(V)$ had eigenvalues 0 or 1, and thus $N(V)$ could not be a projection (assuming that every unit vector in $\mathcal{H}$ represents a physically realizable state).

(2) One can rephrase the spectral conditions in Theorems 2.1 and 2.2 as follows. Consider the intersection $S_k$ of the slab $I_k\times R^3$ with the energy-momentum spectrum. Then Theorem 2.1 requires that the projection of $S_k$ on $R^3$ contain a hole, while Theorem 2.2 requires that it be contained in a ball. This makes it obvious that the spectral assumptions of Theorem 2.2 are stronger than those of Theorem 2.1. However, they are still quite gener-

al. For instance, if $H$ is a continuous function of $|\underline{P}|, H=\omega(|\underline{P}|)$, it is sufficient (but not necessary) that $\omega$ is strictly increasing. If one only has $H \geq f(\underline{P})$ for some (continuous) function $f$, it suffices that $f(\underline{p}) \to \infty$ uniformly as $|\underline{p}| \to \infty$. This covers relativistic systems with $p^0 \geq |\underline{p}|$.

(3) If $H$ is not bounded from below, but otherwise the same spectral conditions hold, one can show by the same argument that for any region $V$ and any state $\psi$ there is a time $t$ such that $\langle U_t\psi, N(V)U_t\psi\rangle \neq 0$, i.e., $U_t\psi$ cannot stay out of $V$ for *all* times.

(4) The conditions on the localization operators $N(V)$ are also quite general. To make this clearer let us first consider a nonrelativistic free particle, with $\mathcal{H}=L^2(R^3, d\underline{x})$. Then $N(V)=\chi_V$, so that

$$\langle\psi, N(V)\psi\rangle = \int \chi_V(\underline{x})|\psi(\underline{x})|^2 d\underline{x} = \int_V |\psi(\underline{x})|^2 d\underline{x}. \quad (2.15)$$

For a relativistic free particle and the Newton-Wigner position operator $\underline{X}_{NW}$, one would have $N(V)=\chi_V(\underline{X}_{NW})$, the projection associated to $V$ in the spectral decomposition of $\underline{X}_{NW}$. Clearly, in both cases conditions (a) and (b) are satisfied.

To get a feeling for the multiparticle case, let us consider a nonrelativistic $N$-particle system with $\mathcal{H}=L^2(R^{3N}, d\underline{x}_1 \cdots d\underline{x}_N)$,

$$\begin{aligned} \underline{P} &= \frac{1}{i}\nabla_1 + \cdots + \frac{1}{i}\nabla_N, \\ H &= -\sum_{i=1}^{N} \frac{1}{2m_i}\Delta_i + \sum_{i<j} U_{ij}(\underline{x}_i - \underline{x}_j). \end{aligned} \quad (2.16)$$

Clearly $H$ and $\underline{P}$ commute. In a center-of-mass system one can write, with $M \equiv \sum_i m_i$,

$$H = \underline{P}^2/2M + \tilde{H}, \quad (2.17)$$

where the first term is the center-of-mass kinetic energy, while $\tilde{H}$ contains only internal variables. If the potentials $U_{ij}$ are such that $\tilde{H}$ is bounded from below the spectral assumptions of Theorems 2.1 and 2.2 are satisfied, since $\underline{p}^2/2M \to \infty$ as $|\underline{p}| \to \infty$. Theorem 2.1 then says that a wave function $\psi(\underline{x}_1, \ldots, \underline{x}_N; t)$ immediately spreads to infinity if initially it has compact support in some or all of its variables.

A localization operator $N(V)$ that satisfies restrictions (a) and (b) is, for instance,

$$N(V) = \chi_V(\underline{x}_i). \quad (2.18)$$

Theorem 2.2 then states that the probability of detecting particle $i$ of the system described by Eq. (2.16) in a given volume cannot vanish for a finite time interval. A similar conclusion holds for the center-of-mass localization operator

$$N(V) = \chi_V\left(\sum_{i=1}^{N} m_i \underline{x}_i / M\right). \quad (2.19)$$

Since the center of mass moves freely, we note that the absence of compact localization and holes in the sense described above can be attributed to the instantaneous spreading of the center-of-mass coordinate.

Setting $N(V)=\chi_V(\underline{x}_1)\cdots\chi_V(\underline{x}_N)$ Theorem 2.2 would seem to lead to the stronger conclusion that the probability of detecting all particles simultaneously in a given volume cannot vanish for any finite time interval. However, this $N(V)$ does not satisfy assumption (b), and so this conclusion is not valid without additional assumptions on the potentials. [See in this connection the first example in Sec. III and the discussion of Eq. (3.15).]

(5) In the case of a relativistic description of particles interacting through pair potentials (as recently studied by one of us[12]) one has $p^0 \geq (\underline{p}^2 + c^2)^{1/2}$, provided the "reduced Hamiltonian" is bounded from below by $c>0$. Thus, the spectral assumptions are satisfied. In this case the operator $N(V)=\chi_V((i/M)\nabla_{\underline{k}})$ satisfies (a) and (b), and may be regarded as the relativistic analog of the center-of-mass operator (2.19) (cf. Ref. 12, Sec. 5.2). However, in spite of the weakness of the restrictions on $N(V)$ it is not clear whether an analog of (2.18) exists that satisfies these restrictions.

## III. SYSTEMS WITH EXTERNAL POTENTIALS

As we have just seen, for many-particle systems it is the spreading of the center of mass that is responsible for the absence of holes. It is therefore a natural question to ask whether similar results can be obtained for the relative motion once the center-of-mass motion is factored out. We shall only address this question for a system of two particles interacting via a pair potential or, equivalently, a particle in an external potential.

As before, we assume the dynamics is given by $U_t = \exp(-iHt)$ on a Hilbert space $\mathcal{H}$, and that the (relative) translations are given by $U(\underline{a}) = \exp(-i\underline{P}\cdot\underline{a})$, $\underline{a} \in R^3$. Moreover, we assume that $H$ is explicitly given by

$$H = H_0 + U, \quad (3.1)$$

where $H_0$ is a function $\omega(\underline{P})$ of the momentum operator $\underline{P}$, while the interaction operator $U$ does not commute with $\underline{P}$.

Without further assumptions on $U$ it can easily happen that the particle stays in a bounded region for all time. To see this, consider the following two examples:

(i) A Schrödinger particle on the line with

$$H = \frac{P^2}{2m} + \chi_{[-1,1]}(x)\frac{1}{1-x^2}. \quad (3.2)$$

The potential has nonintegrable singularities at ±1, so that wave functions in the domain of $H$ must vanish at $x=\pm 1$, while their derivatives may be discontinuous (Dirichlet boundary conditions). As a result, $H$ commutes with $\chi_{[-1,1]}(x)$, so that any wave function with support in $[-1,1]$ will remain in this interval for all time: the particle is "boxed in." Clearly, initial states to the left and right of the box shall also remain there for all time.

(ii) A Schrödinger particle in a space of arbitrary dimension, described by

$$H=\frac{P^2}{2m}-\left\langle g,\left(\frac{P^2}{2m}+1\right)g\right\rangle^{-1}\left|\left(\frac{P^2}{2m}+1\right)g\right\rangle\left\langle\left(\frac{P^2}{2m}+1\right)g\right|, \tag{3.3}$$

has an eigenstate $\psi=g$ with eigenvalue $-1$. If $g$ is a function of compact support, $U_t\psi=\exp(it)\psi$ is always zero outside a fixed bounded region.

These examples show that bound states may be compactly localized for all time; the first example also shows that scattering states may exhibit holes for all time, if the potential is very repulsive. However, a scattering state $\psi$ is a vector in the range of the Møller or wave operators $W_\pm$,

$$\psi=W_{+(-)}\phi=\underset{t\to+\infty(-\infty)}{\text{s-lim}}\exp(iHt)\exp(-iH_0t)\phi \tag{3.4}$$

for some $\phi$, and so $\psi_t$ looks like a freely evolving vector in the future (or past, respectively). In ordinary nonrelativistic quantum mechanics with the usual localization notion, a free state eventually moves out of any finite volume, so for this case also a scattering state should spread to infinity. But there seems to be no physical reason to expect this spreading to be instantaneous. For more general free dynamics and localization notions, as in Sec. II, we have not even shown that a free wave packet eventually leaves every finite volume, so in this general context a scattering state might, conceivably, not spread at all. It may therefore be surprising that also scattering states instantaneously spread to infinity under the same weak hypotheses as in Sec. II B. This is shown in the next result, which is the analog of Theorem 2.1.

*Theorem 3.1* ("instantaneous spreading for scattering states"). Let $H=H_0+U\geq -c$ with $H_0=\omega(\underline{P})$, where the continuous function $\omega$ is not identically constant and is bounded from below. Let $\psi$ be a scattering state as in Eq. (3.4). Finally, assume that

$$\langle U_{t'}\psi, U(\underline{a})U_t\psi\rangle=0\,,\quad \forall\,|\underline{a}|\geq r>0\,,\quad \forall\, t,t'\in[0,\epsilon)\,. \tag{3.5}$$

Then $\psi=0$. If $\omega$ is not bounded from below the conclusion is valid if Eq. (3.5) holds for all $t,t'\in R$.

*Proof.* Since $H\geq -c$, Eq. (3.5) holds for all $t,t'\in R$ by the lemma. Since $\exp(-iH_0t)$ commutes with $U(\underline{a})$ we can write Eq. (3.5) as

$$\langle\exp(iH_0t')\exp(-iHt')\psi, U(\underline{a})\exp[iH_0(t'-t)]\exp(iH_0t)\times\exp(-iHt)\psi\rangle=0,\quad \forall\,|\underline{a}|\geq r\,,\quad \forall\, t,t'\in R\,. \tag{3.6}$$

Now by Eq. (3.4) the vector $\exp(iH_0t)\exp(-iHt)\psi$ strongly converges to $\phi$ for $t\to+\infty(-\infty)$. Hence, putting $t=t'+\tau$ and letting $t'\to+\infty(-\infty)$ in Eq. (3.6) while keeping $\tau$ fixed we obtain

$$\langle\phi, U(\underline{a})\exp(-iH_0\tau)\phi\rangle=0\,,\quad \forall\,|\underline{a}|\geq r\,,\quad \forall\tau\in R\,. \tag{3.7}$$

However, since $\omega(\underline{p})$ is nonconstant and bounded from below all conditions of Theorem 2.1 are met, so that we may infer that $\phi=0$. But then $\psi=0$ by Eq. (3.4). As before, the last assertion follows trivially by starting directly from Eq. (3.6). Q.E.D.

As the preceding two examples show, this result cannot be carried over to the "no holes" case. In the Appendix we will prove a similar result for any vector in the continuous spectrum of $H$.

To investigate the spreading of an arbitrary state $\psi\in\mathcal{H}$ we can decompose it into a superposition of bound states and a scattering state[13] and consider these states separately. This is seen as follows. Let $U_t=\exp(-iHt)$ with $H\geq -c$ and assume that for some $\psi\in\mathcal{H}$ and some $V$

$$\langle U_t\psi, N(V)U_t\psi\rangle=0 \quad\text{for all } t\in[0,\epsilon]\,.$$

By the lemma this holds for all $t\in R$, and thus

$$N(V)U_tU_\tau\psi=0\,,\quad \forall\, t,\tau\in R\,.$$

From this we conclude for any interval $I$,

$$N(V)U_t\chi_I(H)\psi=0\,,\quad \forall\, t\in R\,.$$

Similarly,

$$\langle\psi, U(\underline{a})U_t\psi\rangle=0\,,\quad \forall\, t\in[0,\epsilon]\,,$$

implies

$$\langle\chi_I(H)\psi, U(\underline{a})U_t\chi_I(H)\psi\rangle=0\,,\quad \forall\, t\in R\,.$$

With $\chi_I(H)$ we can project out any part of the spectrum, in particular the bound states. Writing

$$\psi=\sum\alpha_i\psi_i+\psi_{\text{scatt}}\,, \tag{3.8}$$

where $\psi_i$ are (normalized) eigenstates of $H$, we conclude that if $\psi$ is not localized in $V$ for $t$ in a finite time interval, then this holds for the $\psi_i$'s and $\psi_{\text{scatt}}$ as well.

It thus remains to consider the localization properties of bound states. General results for these are only known for Schrödinger operators $H=-\Delta/2m+U$. For a large class of potentials it is known that eigenfunctions of $H$ cannot vanish on open sets.[14] For the time-dependent Schrödinger equation for $N$ particles with

$$H=\sum_j [-i\nabla_j-\underline{A}_j(x)]^2+U(\underline{x}_1,\ldots,\underline{x}_N)\,, \tag{3.9}$$

where $H \geq -c$ and where $\underline{A}_j$ and $U$ satisfy some technical conditions, it is known that a solution $\psi(\underline{x}_1,\ldots,\underline{x}_N;t)$ cannot vanish on an open space-time set unless it vanishes identically.[15] For the Klein-Gordon equation with external potentials a similar result is known.[16] It should be noted, however, that the space variable $\underline{x}$ in the Klein-Gordon equation is not a position variable as in the Schrödinger case, so that the relevance of Ref. 16 with respect to particle localization is not obvious.

The results of Refs. 14–16 depend on detailed properties of partial differential equations and do not allow for more general localization notions. It would therefore be interesting to find general conditions on non-translation-invariant Hamiltonians that lead to results similar to those of Sec. II.

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## APPENDIX

From an operator-theoretic point of view the spectral assumptions we made in Theorem 2.1 [2.2] were used to prove the following two facts: If $\psi\in\mathcal{H}$ and $A$ is some bounded operator on $\mathcal{H}$, then the assumption

$$AU(\underline{a})U_t\psi=0 \tag{A1}$$

for any $t$ in a nonzero time interval and any $\underline{a}\in R^3$ with $|\underline{a}|\geq r$ $[|\underline{a}|\leq r]$ $(r>0)$ implies that

$$AU(\underline{a})\psi=0\,,\quad \forall\,\underline{a}\in R^3\,. \tag{A2}$$

Indeed, in the proofs of these theorems we took $A=|\psi\rangle\langle\psi|$ $[A=N(V')]$, and an inspection of the proofs shows that the spectral assumptions were only used to get (A2) from the assumption (A1).

We shall now restate and rigorously prove these two facts under even weaker spectral assumptions on the generators $H$ and $\underline{P}$. We denote by $D_E$ and $M_{\underline{p}}$ the spectral families of the dynamics $H$ and momentum $\underline{P}$, in terms of which $U_t$ and $U(\underline{a})$ can be written as

$$U_t=\int \exp(-itE)dD_E\,, \tag{A3}$$

$$U(\underline{a})=\int \exp(-i\underline{p}\cdot\underline{a})dM_{\underline{p}}\,. \tag{A4}$$

We shall denote the spectral projections of $H$ and $\underline{P}$ corresponding to measurable sets $\Lambda\subset R$ and $\Omega\subset R^3$ by $D_\Lambda$ and $M_\Omega$, respectively. The conditions (A5), (A6) and (A5), (A13) below correspond to the spectral assumptions of Theorems 2.1 and 2.2, respectively.

*Theorem A.1* ("no compact localization"). Assume there exists a sequence of sets $\Lambda_k\subset R$ and a sequence of sets $\Omega_k\subset R^3$ with nonzero Lebesgue measure $(k=1,2,\ldots)$, satisfying

$$\operatorname*{s-lim}_{N\to\infty}\sum_{k=1}^N D_{\Lambda_k}=1 \tag{A5}$$

and

$$M_{\Omega_k}D_{\Lambda_k}=0\,,\quad k=1,2,\ldots\,. \tag{A6}$$

Assume moreover that (A1) holds for any $t\in R$ and any $\underline{a}\in R^3$ with $|\underline{a}|\geq r>0$. Then (A2) holds true.

*Proof*. The assumptions imply that for any $\phi\in\mathcal{H}$ one has

$$\langle\phi,AU(\underline{a})U_t\psi\rangle=\int\exp(-itE)d_E\langle\phi,AU(\underline{a})D_E\psi\rangle=0\,,$$
$$\forall t\in R,\quad \forall\,|\underline{a}|\geq r\,. \tag{A7}$$

Hence, the measure $d_E\langle\phi,AU(\underline{a})D_E\psi\rangle$ vanishes for $|\underline{a}|\geq r$, so that

$$\langle\phi,AU(\underline{a})D_{\Lambda_k}\psi\rangle=0\,,\quad k=1,2,\ldots,\quad \forall\,|\underline{a}|\geq r\,. \tag{A8}$$

Using (A4) we have

$$\begin{aligned}F_k(\underline{a})&\equiv\langle\phi,AU(\underline{a})D_{\Lambda_k}\psi\rangle\\&=\int\exp(-i\underline{p}\cdot\underline{a})d_{\underline{p}}\langle\phi,AM_{\underline{p}}D_{\Lambda_k}\psi\rangle\,,\quad k=1,2,\ldots\,.\end{aligned} \tag{A9}$$

By virtue of (A8) the functions $F_k$ have compact support, so that their Fourier transforms $\tilde{F}_k$ are real-analytic. As a result we can write

$$d_{\underline{p}}\langle\phi,AM_{\underline{p}}D_{\Lambda_k}\psi\rangle=\tilde{F}_k(\underline{p})d\underline{p}\,, \tag{A10}$$

where $d\underline{p}$ denotes Lebesgue measure. If one integrates this equality over any subset of $\Omega_k$, the left-hand side vanishes by assumption (A6), implying that $\tilde{F}_k(\underline{p})$ vanishes on $\Omega_k$. But $\Omega_k$ has nonzero Lebesgue measure and $\tilde{F}_k$ is real-analytic, so that $\tilde{F}_k$ vanishes identically. Hence,

$$\langle\phi,AU(\underline{a})D_{\Lambda_k}\psi\rangle=0\,,\quad k=1,2,\ldots\,,\quad \forall\,\underline{a}\in R^3\,, \tag{A11}$$

so that by assumption (A5)

$$\langle\phi,AU(\underline{a})\psi\rangle=0\,,\quad \forall\,\underline{a}\in R^3\,. \tag{A12}$$

Since $\phi$ was arbitrary this implies (A2). Q.E.D.

*Theorem A.2* ("no holes"). Assume there exists a sequence of sets $\Lambda_k\subset R$ and a sequence of compact sets $C_k\subset R^3$ satisfying (A5) and

$$M_{C_k}D_{\Lambda_k}=D_{\Lambda_k}\,,\quad k=1,2,\ldots\,. \tag{A13}$$

Assume, moreover, that (A1) holds for any $t\in R$ and any $\underline{a}$ in some set $\Omega\subset R^3$ with nonzero Lebesgue measure. Then (A2) holds true.

*Proof*. Arguing as in the proof of Theorem A.1

one infers that the functions

$$F_k(\underline{a}) \equiv \langle \phi, AU(\underline{a})D_{\Lambda_k}\psi\rangle = \int \exp(-i\underline{p}\cdot\underline{a})d_{\underline{p}}\langle\phi, AM_{\underline{p}}D_{\Lambda_k}\psi\rangle \quad (A14)$$

vanish for $\underline{a}\in\Omega$. Now from (A13) it follows that

$$F_k(\underline{a}) = \int_{C_k} \exp(-i\underline{p}\cdot\underline{a})d_{\underline{p}}\langle\phi, AM_{\underline{p}}D_{\Lambda_k}\psi\rangle. \quad (A15)$$

But $C_k$ is compact, so that $F_k$ is real-analytic. Since $\Omega$ has nonzero Lebesgue measure it follows that $F_k$ vanishes identically. But then one has, using (A5),

$$\langle\phi, AU(\underline{a})\psi\rangle = \lim_{N\to\infty}\sum_{n=1}^{N}\langle\phi, AU(\underline{a})D_{\Lambda_k}\psi\rangle = 0, \quad \forall \underline{a}\in R^3, \quad (A16)$$

from which (A2) follows. Q.E.D.

*Remarks.*

(1) If one assumes in addition that $H$ is bounded from below, Eq. (A1) need only hold for $t$ in a nonzero time interval by the lemma.

(2) The assumption (A13) is stronger than (A6). Indeed, if (A13) holds one can take for $\Omega_k$ the complement of $C_k$. Since $C_k$ is compact, $\Omega_k\equiv R^3\backslash C_k$ has nonzero Lebesgue measure, and one also has $M_{\Omega_k}D_{\Lambda_k} = (1-M_{C_k})D_{\Lambda_k} = 0$ by (A13).

We close this appendix by showing that instantaneous spreading occurs for any state in the continuous spectrum of a semibounded Hamiltonian $H$ of the form (3.1), provided some technical assumptions are met. We assume that $\mathcal{H} = L^2(R^3, d\underline{x})$, $\underline{P} = (1/i)\nabla$, and $H_0 = \omega(\underline{P})$. As is well known, $\mathcal{H}$ can be written as a direct sum of subspaces

$$\mathcal{H} = \mathcal{H}_{\text{p.p.}} \oplus \mathcal{H}_{\text{s.c.}} \oplus \mathcal{H}_{\text{a.c.}} \quad (A17)$$

containing vectors $g$ for which the measure $d_E(g, D_E g)$ is discrete (i.e., bound states), singular continuous, and absolutely continuous.

*Theorem A.3* ("instantaneous spreading for states in the continuous spectrum"). Assume that $\psi$ is orthogonal to $\mathcal{H}_{\text{p.p.}}$ and that

$$\chi_C U_t\psi = U_t\psi \quad (A18)$$

for some compact set $C$ and any $t$ in a nonzero time interval. Assume, moreover, that $H$ has the same domain as $H_0 = \omega(\underline{P})$, and that the function $\omega$ is bounded from below, and such that $(\omega(\underline{p})+i)^{-N}$ is square-integrable for some $N\geq 1$. Then $\psi = 0$.

*Proof.* By the lemma, (A18) holds for any $t\in R$. For $\psi\in\mathcal{H}_{\text{a.c.}}$ the assertion can then be shown by the following argument: As is well known, one has

$$\operatorname*{w-lim}_{t\to\pm\infty} U_t\phi = 0 \quad (A19)$$

for any $\phi\in\mathcal{H}_{\text{a.c.}}$ by the Riemann-Lebesgue lemma. We now claim that $\chi_C(H+i)^{-1}$ is a compact operator. Taking this for granted, it follows from this and (A19) that

$$\operatorname*{s-lim}_{t\to\pm\infty} \chi_C U_t\phi = 0 \quad (A20)$$

for any $\phi\in\mathcal{H}_{\text{a.c.}}\cap D(H)$, and therefore by a density argument for any $\phi\in\mathcal{H}_{\text{a.c.}}$, in particular for $\psi$. But since (A18) holds for any $t\in R$ it then follows that $\psi = 0$, as claimed.

To prove the compactness assertion, we note that it suffices to show that $\chi_C(H+i)^{-1}$ is compact. Indeed, since $H_0$ and $H$ have the same domain, the operator $(H_0+i)(H+i)^{-1}$ is bounded by the closed-graph theorem. But $\chi_C(\underline{x})$ is in any $L^q(R^3, d\underline{x})$ since $C$ is compact, while $(\omega(\underline{p})+i)^{-1}$ is in $L^q(R^3, d\underline{p})$ for $q\geq 2N$. Therefore, $\chi_C(H_0+i)^{-1}$ belongs to the trace ideal $\mathcal{I}^q$ for $q\geq 2N$,[17] and in particular is compact.

To prove the theorem in the general case we combine the "RAGE" theorem[18] with the argument given above: since $\chi_C(H+i)^{-1}$ is compact, the RAGE theorem implies that

$$\frac{1}{2T}\int_{-T}^{T}\|\chi_C\exp(-iHt)\psi\|^2 \xrightarrow[T\to\infty]{} 0 \quad (A21)$$

for $\psi\in\mathcal{H}_{\text{s.c.}}\oplus\mathcal{H}_{\text{a.c.}}$. But in view of (A18) this can only hold if $\psi = 0$. Q.E.D.

*Remarks.*

(1) If $\omega$ is not semibounded, but the assumption (A18) holds for any $t\in R$, the conclusion of the theorem is still valid.

(2) The assumptions of the theorem also imply the following conclusions, as the proof shows: States in $\mathcal{H}_{\text{a.c.}}$ move out of any finite volume in the distant past and future [by Eq. (A20)], while states in $\mathcal{H}_{\text{s.c.}}$ do so in the average sense of Eq. (A21). Thus, such states always tunnel out of potential wells of arbitrary shape and depth.

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*On leave from the Institut für Theoretische Physik, Universität Göttingen.

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[6]This can be formulated rigorously in terms of direct

integrals.

[7]See, e.g., N. Levinson and R. M. Redheffer, *Complex variables* (Holden-Day, San Francisco, 1970).

[8]Note that $f(H)=\int \tilde{f}(t)\exp(iHt)\,dt$, where the Fourier transform $\tilde{f}$ of $f$ is a continuous function.

[9]$\psi_k(\underline{p})$ will in general be a multicomponent function.

[10]In this case there is a number $E$ such that on the momentum spectrum $\omega$ takes values both in $I_1=[-c,E)$ and in $[E,\infty)$. Hence $\omega^{-1}(I_1)$ contains only a part of the momentum spectrum, and thus there is a set $0_1$ with $I_1 \times 0_1$ not in the energy-momentum spectrum. Dividing $[E,\infty)$ into a union of finite disjoint intervals $I_k$, $k=2, \cdots$, the same argument can be repeated.

[11]This means that if the energy is in $I_k$ the momentum has to be in $B_k$.

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[13]At this point we assume for simplicity that each state is such a superposition (asymptotic completeness). The mathematically more complete case with discrete, absolutely continuous and singular continuous spectrum is treated in the Appendix.

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